



chain nodes :

7 8 9 10 11 12 13 14 15 16 23 24 25 26 27 28 29 30 31

ring nodes :

1 2 3 4 5 6

chain bonds :

4-8 5-7 7-23 8-9 10-11 11-12 13-14 14-15 14-16 24-25 26-27 28-29 30-31

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

4-8 5-7 7-23 8-9 10-11 11-12 13-14 14-15 14-16 28-29 30-31

exact bonds :

24-25 26-27

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

G1: [*1], [*2]

G2: Cy, Ak

G3: H, S, [*3], [*4], [*5], [*6]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 23:CLASS 24:CLASS 25:CLASS
 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS